

Day 1: Finite Temperature Properties of Materials and Molecules

Thursday, October 13th, 2022

Morning Session: Argonne National Laboratory, Building 240, Room 1501

8:45—9:00	Welcome Note and Introduction (15 min) <i>Giulia Galli</i>
9:00—10:00	Lecture: First Principles Molecular Dynamics (1h) <i>Francois Gygi</i>
10:00—10:30	Coffee Break (30min)
10:30—12:00	Tutorial: First Principles Molecular Dynamics with Qbox (1h30min) <i>Francois Gygi</i>
12:00—12:30	Break (30 min) Group picture

Afternoon Session: Argonne National Laboratory, Building 241, Room D172

12:30—1:30	Working Lunch (meal provided) (1h) Lecture: Advanced Sampling Techniques <i>Jonathan Whitmer</i>
1:30—3:00	Tutorial: Free-energy Calculations of Defects with the Qbox-SSAGES coupling (1h30min) <i>Elizabeth Lee & Cunzhi Zhang</i>
3:00—3:30	Coffee Break (30min)
3:30—5:00	Free-energy calculations with pySAGES (1h30min) <i>Pablo Zubieta</i>

Day 2: Computational Spectroscopy

Friday, October 14th, 2022

Morning Session: Argonne National Laboratory, Building 240, Room 1501

9:00—10:00	Lecture: Computational Spectroscopy (1h) <i>Giulia Galli</i>
10:00—10:30	Coffee Break (30min)
10:30—12:00	Tutorial: Photoemission Spectra with WEST (1h30min) <i>Marco Govoni & Victor Yu</i>
12:00—12:30	Break (30 min)

Afternoon Session: Argonne National Laboratory, Building 241, Room D172

12:30—1:30	Working Lunch (meal provided) (1h) Lecture: Simulation of Photoluminescent Spectra <i>Yu Jin</i>
1:30—3:00	Tutorial: Quantum Defect Embedding Theory (1h30min) <i>Christian Vorwerk & Marco Govoni</i>
3:00—3:30	Coffee Break (30min)
3:30—5:00	Tutorial: Spin Coherence with pyCCE (1h30min) <i>Nikita Onizuk</i>